

# MECHANISM OF THERMAL DECOMPOSITION OF BISPHENOL C

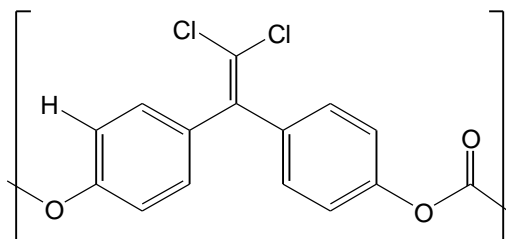
## POLYCARBONATE: NATURE OF ITS FIRE RESISTANCE

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**ABSTRACT:** Bisphenol C Polycarbonate (BPC PC, see Figure 1) is one of the most fire-resistant polymer known to the scientific community. At the same time, this material has mechanical properties that make it suitable for transportation applications requiring toughness and durability.<sup>1</sup> According to the experimental analysis,<sup>1,2</sup> thermal degradation of BPC PC leads to formation of high amounts of char (50 % by weight) and non-flammable gaseous products, CO<sub>2</sub> and HCl. These experimental observations provide a direct explanation of the exceptional fire resistance of this material. However, the chemical mechanism that is responsible for the formation of these decomposition products is not understood.



**Figure 1. Structure of BPC PC.**

In this study, B3LYP<sup>3</sup> density-functional method was employed for analysis of reaction pathways of thermal decomposition of BPC PC. On the bases of the computational results, a mechanism of thermal decomposition of this polymer was proposed. According to the mechanism, the decomposition occurs via formation of Cl-atom – Phenyl ring complexes, which provide weak crosslinks between the polymer chains at initial stages of the process. These complexes, subsequently, decompose via elimination of HCl. The radical sites, formed as a result of these reactions, recombine forming strong covalent bonds between bisphenol fragments of the polymer chains. The process of crosslinking (which eventually leads to the formation of char) competes with the process of backbone cleavage, which also leads to the formation of CO<sub>2</sub>. The proposed mechanism provides a plausible explanation of the numerous experimental observations.<sup>1,2</sup>

### References:

1. Ramirez M. L. *M.S. Thesis*; University of Puerto Rico; **2000**.
2. Stewart, J. *Ph.D. Dissertation*; University of Massachusetts, Amherst; **1999**.
3. Becke, A. D. *J. Chem. Phys.* **1992**, 97: 9173.

